

On the macroscopic free energy potential for Shape Memory Alloys treated as a two-phase continuum

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IN THE PRESENT PAPER, a macroscopic free energy potential for shape memory alloys in the pseudoelastic range of their behavior is derived. It is assumed that the macro-element made of Shape Memory Alloy (SMA) is composed of austenitic and martensitic phase. It is stipulated that on the mezo-scale level, the micro-constituents obey generalized thermoelastic Hooke's law, in which eigenstrains connected with martensitic phase transformation are present. The primary target of the paper is not determination of the specific form of the macro free energy but revealing its structure resulting from the micro-macro transition. This structure is of a fundamental significance for subsequent development of macroscopic constitutive relations for Shape Memory Alloys. Micro-macro transition procedure allows for identifying the correspondence between the actual micro-phenomena and individual terms appearing in the free energy macro-potential. The performed calculations throw a new light on the so-called accommodation energy, a part of which is the interaction (coherence) energy appearing in contemporary literature. On the application side, it was possible to explain a certain paradox appearing in the attempts made to describe the behavior of some TiNiX ternary alloys (TiNi alloy) undergoing R-phase transformation.

1. Introduction

RECENTLY MUCH ATTENTION in research and industry has been focused on materials, which exhibit properties unusual in comparison to "standard" materials. These materials can further be used for construction of smart structures (see e.g. [22]). Shape memory alloys such as NiTi, TiNiCo, TiNiAl, CuZnAl, CuAlNi are prime candidates here. They are already used in construction of connectors, release mechanisms, control devices, medical tools and many other engineering mechanisms (see [14]). What makes the shape memory alloys special is that they can fully recover from relatively large strains (on the level of 4% – 8% in practical applications) upon appropriate stress and/or temperature histories. Metallurgical studies showed that this special effect of SMA materials originates from the thermoelastic martensitic transformation (see e.g. [12]). During this transforma-

tion, a high temperature and high symmetry austenitic phase of SMA transforms into a low temperature and lower symmetry martensitic phase. The transformation may be induced either by lowering temperature or applying stress. The microstructures appearing as a result of this transformation were extensively investigated in metallurgical literature during the last forty years and are at present quite well known. For an extensive review of the thermoelastic martensitic transformation and microstructure properties arising from the metallurgical point of view we shall send the reader to the book by CHRISTIAN [3] and his very recent paper [2]. The theoretical works aiming at the description of shape memory alloys behavior lagged behind the experimental ones until late 80-ties and beginning of the 90-ties when a number of models of SMA materials mechanical behavior appeared. Apparently, FALK [4] has proposed the first macroscopic thermodynamic constitutive model of SMA materials. He postulated the free energy potential in the form of a 6th degree polynomial. He managed to obtain a good qualitative description of SMA materials in pseudoelastic range of their behavior, without introducing any internal variables in his model. The coherence energy Φ^{AM} proportional to the product of martensitic phase and austenitic phase fraction made a big step in modeling of Shape Memory Alloys. This term introduced heuristically into the free energy potential allowed for a good quantitative description of the hysteresis loop formation on the grounds of non-equilibrium thermodynamics.

Many researchers have adopted this approach, e.g. Müller and his collaborators managed to model successfully the macroscopic behavior of shape memory alloys subjected to one-dimensional mechanical loading ([10], [6]). RANIECKI, LEXCELLENT and TANAKA [18], [17] developed the so-called R_L incremental macroscopic model. The model is three-dimensional and allows for arbitrary thermo-mechanical loading. The typical behavior of CuZnAl mono-crystalline sample during isothermal uniaxial tension is sketched in Fig. 1. The σ_1^{AM} denotes the critical stress of forward transformation, σ_1^{MA} denotes the critical stress of reverse transformation, γ is the amplitude of pseudoelastic flow at simple tension. This behavior may be easily reproduced with the aid of the R_L model. The dashed line shows the states of full thermodynamic equilibrium predicted by this model. It may be shown that the equilibrium is unstable when $\Phi^{AM} > 0$ and this explains, on a theoretical ground, the formation of the hysteresis loop as discussed in [18]. It was also shown in [18] that $\Phi^{AM} > 0$ when $\sigma_1^{AM} > \sigma_1^{MA}$.

The R_L model has been adopted in [7] for description of the R-phase transformation. However, in this case $\sigma_1^{AM} < \sigma_1^{MA}$, what is shown schematically in Fig. 2. Identification of the macroscopic constitutive model material parameters leads to negative values of the term Φ^{AM} . The negative value of interaction energy Φ^{AM} constitutes a paradox and deserves further investigation. The dashed line in Fig. 2 shows the states of full thermodynamic equilibrium predicted by the model. Deviation of the real paths from the paths of full thermodynamic equi-

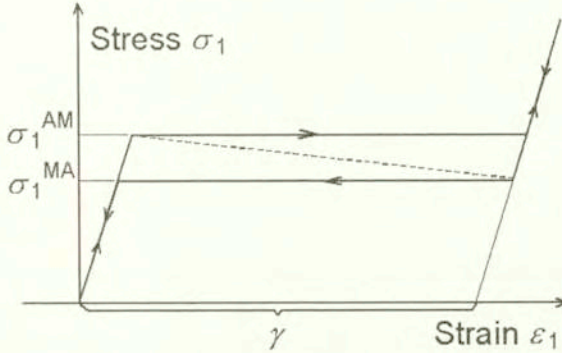


FIG. 1. Typical behavior of CuZnAl alloy.

librium can not be explained anymore by its instability. LIM and MCDOWELL performed experimental works on NiTi samples and presented the discussion devoted to the interaction energy Φ^{AM} in [8]. At the end of their paper they propose that the interaction energy should be a function of temperature, internal variables and phase fractions, but not necessarily proportional to their product. They do not lead to any specific explicit expression for the interaction energy.

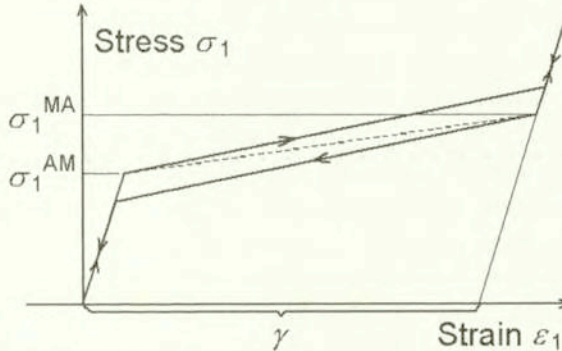


FIG. 2. Typical behavior of TiNi alloy undergoing R-phase transformation.

The present paper is an attempt to analyze the fundamental problem of the general structure of macroscopic free energy potential enabling the description of SMA materials. We are not trying at the same time to construct here a new or revised micro-mechanical or macroscopic constitutive model of SMA materials. The procedure applied to construct such a model when the free energy potential is already known is clearly indicated in papers [17] and [18]. We will start our investigation from the so-called mezo-scale of observation. All our starting mezo-scale assumptions will be supported by metallurgical observations on this scale. We will postulate elastic behavior of both phases on this scale of observation. It

is worth noticing that even when the particular micro-constituents of the macro-element behave elastically, the overall response of the material may be non-elastic and possibly dissipative. The reason for that is the evolving microstructure in the RVE (phase transformation or reorientation of martensitic variants) and usually the accompanying it phenomenon of energy dissipation.

We will not investigate these issues in the present paper, sending interested readers to the papers by ABEYARATNE and KNOWLES [1] or RANIECKI and TANAKA [19]. We are studying an arbitrary but fixed instant of the phase transformation progress. The macro-element is assumed to be in the thermodynamic equilibrium with respect to the external thermodynamic variables (macroscopic strain $\boldsymbol{\varepsilon}^{(z)}$ and temperature T). Constrained thermodynamic equilibrium is postulated with respect to the parameters describing the microstructure of macro-element \mathbf{H} . One of the simplest parameters of this kind is the mass fraction of martensitic phase z . Hence, all the theorems of the theory of elasticity will be valid in our considerations.

Later, taking into account the changing microstructure of the RVE or phase fraction z will result in changing the eigenstrains of the phase transformation, but will not result in a change of the general structure of free energy macro-potential. As a result of our mezo-macro transition procedure, we will obtain free energy expressed in terms of macro-state variables understood as relevant averaged values of the corresponding mezo-variables. We will not solve the mezo-mechanical problem explicitly, as this would require prescribing a fixed RVE microstructure. The microstructures observed in real samples are pretty complex and finding analytical solutions for them might be extremely difficult. Nevertheless, we will obtain the sought structure of the free energy macro-potential. The particular terms appearing there may be interpreted in terms of the underlying mezo-scale phenomena and mezo-scale variables. The wealth of alloys exhibiting shape memory effects indicate that some terms appearing in the free energy macro-potential derived from mezo-mechanical assumptions may be neglected for some alloys but not for the others. Also the observation of macroscopic behavior of certain SMA materials allows drawing the conclusion that some microscopic phenomena do not take place there. For example, ideal pseudoelastic flow will indicate the formation of martensitic plates without complex internal microstructure (composed e.g. of one martensitic variant). Strong work-hardening observed during the R-phase transformation indicates the formation of many martensitic plates with internal substructure. Several authors tried to derive constitutive relations for the SMA materials starting from micro-mechanical considerations; see, e.g. papers by PATOOR *et. al.* [13] or SUN *et. al.* [20]. The authors mentioned above concentrated on deriving the "working" constitutive models of SMA materials. They were not concentrating to a large extent on the macroscopic free energy macro-potential itself.

2. Thermoelastic martensitic transformation experimental evidence in mezo-scale of observation

The most important information from metallurgical literature concerning thermoelastic martensitic transformation is shortly recalled in the present section. The information specified below is necessary for a proper choice of mezo-scale variables (and their properties) appearing in the mezo-scale mechanical problem posed in the subsequent sections. Various patterns of martensitic structure appearing on subsequent levels of observation are illustrated schematically in Figs. 3 to 6. In the materials science literature devoted to martensitic transformations, e.g. CHRISTIAN [3], OLSON and OWEN [12] or WARLIMONT, DELAËY [21], the following properties characteristic for martensitic transformations could be found:

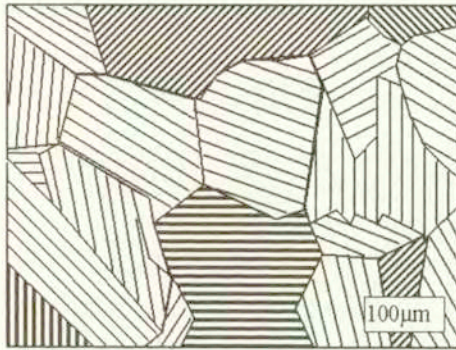


FIG. 3. Schematic view of polycrystalline martensitic microstructure in Cu-Al. Observe different orientation of martensitic plates in different grains (after WARLIMONT and DELAËY [21]).

a) Martensitic phase transformation is athermal, i.e. it does not depend on the time and the rate of change of parameters inducing it.

b) Martensitic transformation is coherent and is also called generalized plane strain transformation since during this transformation the planes are formed, which remain invariant (not deformed and not rotated). They are called habit planes, and constitute a border between the parent and product phases. The atoms, which actually take part in transformation, move in the same direction by a distance proportional to the distance from the habit plane.

c) Martensitic transformation is diffusionless, i.e. chemical composition of the parent and martensitic phase is the same.

d) Thermoelastic martensitic transformation is shear strain dominant displacive transformation progressing by nucleation and growth, where shear strains can reach about a dozen percent while the bulk strain is very limited (max. up to 0.5%) [12].

e) Typical generic element of thermoelastic martensite structure is a thin plate or a thin lens (see Fig. 4). The martensitic plate has usually an internal microstructure itself composed of twin martensitic variants (see Fig. 5)).

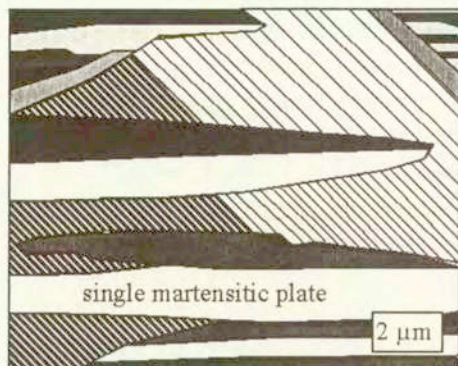


FIG. 4. Schematic view of formation of groups of martensitic plates (after WARLIMONT and DELAEY [21]).

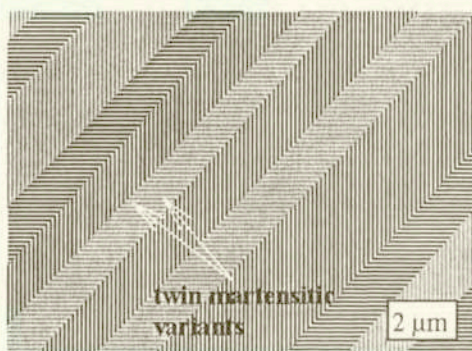


FIG. 5. Schematic view of internal microstructure of martensitic plates (after WARLIMONT and DELAEY [21]).

f) Thermoelastic martensite may be induced thermally or mechanically.

g) The martensitic phase usually has an internal hierarchical microstructure. On the higher level it consists of many martensitic plates. They in turn may consist of several martensitic variants. For example, the martensite induced thermally has usually the microstructure with groups of four self-accommodating martensitic variants. On the other hand, the martensite induced by or at the presence of stress has the microstructure with martensitic variants of preferred orientation with respect to the applied stress direction (see, e.g. PUTAUX and CHEVALIER [16]). This last feature allows proposing a macroscopic constitutive relation between the external stress tensor $\sigma^{(z)}$ and the phase transformation eigenstrain tensors.

The above experimental evidence known from the metallurgical literature will be analyzed in the next section from the point of view of continuum thermo-mechanics. The issue of phase transformation kinetics is not touched in the present paper. The reason for that is that the macro-element of the Shape Memory Alloy is investigated in the present paper at a fixed point of the phase transformation progress. This means that the investigations in the present work are limited to a generalized problem of elasticity. The approach is quite similar to that applied in the problems of homogenization of composites, when the primary task is the determination of the effective moduli.

3. Continuum mechanics approach to thermo-elastic martensitic transformation

In the present section we are studying thermo-elastic martensitic transformation properties from the point of view of continuum thermo-mechanics. This will enable us to adopt suitable mezo-scale variables with properties adequate for the description of the shape memory alloys behavior. The properties of mezo-scale variables identified hereby on the basis of experimental evidence will translate to macro-variables through the averaging procedure. In our investigation we will use the postulate of local state, saying that the behavior of the material in a material point is predetermined by its closest neighborhood, the so-called Representative Volume Element - RVE (see Fig. 6). On the level of RVE, the mezo-scale variables depend on spatial coordinate x . The averaging procedure carried out over the volume of RVE will result in the value of macroscopic variable in the material point.

The property a) of the previous section on the mezo- and macro- scale of observation must result in the rate-independence of the constructed constitutive model of shape memory alloy. This is the assumption made in the present paper, which finds its reflection in the independence of the phase mezo-scopic potentials adopted in the next section from the rates of state parameters. They depend only on the state parameters themselves. It also suggests construction of rate-independent phase transformation kinetic equations, which are not discussed here.

In the property b) it is said that the martensitic transformation is coherent. This means that the field of displacements appearing in the continuum mechanics problem must be continuous, but not the strains field, which may be discontinuous on the phase boundaries. The second part of property b) allows us to draw a conclusion that the gradient of deformation \mathbf{F}_2 in a single martensitic plate can be expressed as $\mathbf{F}_2 = \mathbf{1} + \boldsymbol{\lambda} \otimes \mathbf{n}$. Where the austenitic phase has been adopted as the reference state ($\mathbf{F}_1 = \mathbf{1}$), $\boldsymbol{\lambda}$ is a vector of martensitic phase distortion,

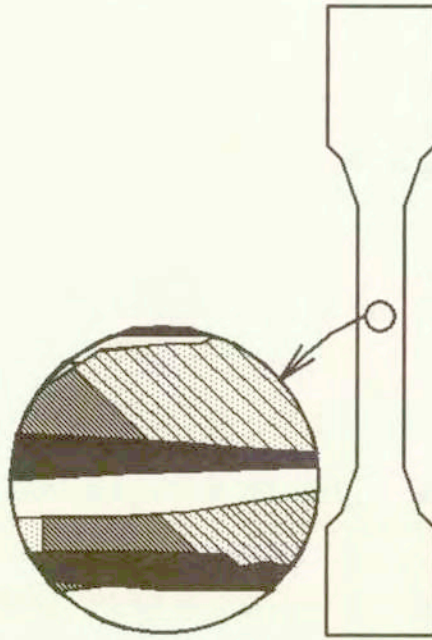


FIG. 6. Representative volume element of SMA.

while \mathbf{n} is a vector normal to the austenite-martensite interface. The volume strain in thermoelastic martensitic transformation does not exceed 0.5%. Hence, it is justified to adopt the approximation that volume and weight fractions of the austenite and thermo-elastic martensite are identical $\rho_1 = \rho_2$. The relation $\det(\mathbf{F}_2)/\det(\mathbf{F}_1) = \rho_1/\rho_2 = 1 + \boldsymbol{\lambda} \cdot \mathbf{n}$ shows how the volumetric strain can be estimated from the measurement of microscopic parameters $\boldsymbol{\lambda}$ and \mathbf{n} .

Also from d) we know that the shear strains observed in SMA materials are limited to a dozen percent or so. In practical applications they usually do not exceed 8%. Hence, it is justified to conduct the present investigations within the framework of the small strains theory. The form of deformation gradient \mathbf{F}_2 specified above is valid, with good reliability, for a single martensitic plate. Metallographic micrographs of martensitic structures indicate (see e.g. [21]) that this simple form of deformation gradient cannot be adopted even on the mezo-scale of observation, unless the evolution of a single martensitic plate or even of a single martensitic variant is studied.

In the present paper it is assumed that the phase transformation eigenstrain tensors are functions of the position in the RVE volume and are not constant. This last assumption is natural in view of the complicated martensitic microstructures resulting from thermoelastic martensitic transformation (see, e.g. Fig. 6). When only single martensitic plate will appear composed of single martensitic

variant, then the transformation eigenstrain is constant. In the case, when one martensitic plate composed of twin alternating martensitic variants then the eigenstrain may be assumed to be constant but with the vector λ different from the previous case. In general, on the meso-scale of observation supposition on non-homogeneous phase transformation eigenstrain is well justified. The non-homogeneity results from formation of many martensitic plates with internal substructure as observations e) and g) indicate.

In the present investigation another important simplifying assumption is made, stating that the tensors of elastic stiffness and elastic compliance of austenitic and martensitic phase \mathbf{L}_α and $\mathbf{M}_\alpha \equiv (\mathbf{L}_\alpha)^{-1}$ ($\alpha = 1, 2$) are material constants independent of the thermodynamic state. The thermal expansion coefficients α , and specific heats c , are material constants and are assumed to be the same for both phases.

The property f) calls for development of the SMA materials theory within the thermodynamical framework. This is actually done in the present paper. It should also find its reflection in the forward and reverse phase transformation criteria as well as in the phase transformation kinetic relations.

4. Formulation of mezo-mechanical boundary value problem of two phase continuum for RVE

In this section we explicitly formulate the problem of mezo-mechanics for representative volume element of shape memory alloy. The problem is posed in meso-scale state variables. When a solution of the problem is known, the explicit form of stress macro-potential may be obtained by "simple" averaging of meso-scale variables over the RVE volume. We already remarked that the martensitic structures appearing in RVE are usually very complex. This practically excludes the possibility to find an analytical solution of the posed problem. The solution derived in the present paper is to a large extent formal one. Nevertheless, it gives useful information on the form of the free energy potential allowable from the point of view of micro-mechanics. It also allows to predict, which macroscopic terms may be neglected in this potential for some microstructures and not for the others.

We will assume that thermoelastic properties of individual phases are described on meso-scale by free energy micro-potentials identical with those adopted in the linear theory of thermo-elasticity. This means that the phases on meso-scale obey generalized Hook's laws,

$$(4.1) \quad \rho\phi_{(\alpha)}(\hat{\hat{\epsilon}}_\alpha(\mathbf{x}, T), T) = 0.5(\hat{\hat{\epsilon}}_\alpha(\mathbf{x}, T) - \hat{\Gamma}_\alpha(\mathbf{x}, T)) \cdot \mathbf{L}_\alpha(\dot{\hat{\epsilon}}_\alpha(\mathbf{x}, T) - \dot{\hat{\Gamma}}_\alpha(\mathbf{x}, T)) + \rho\phi_{(\alpha)}^0(T),$$

$$(4.1) \quad \rho\phi_{(\alpha)}^0(T) = c[T - T_0 - T \ln(T/T_0)] + \left(u_0^{*(\alpha)} - T_{s_0}^{*(\alpha)} \right),$$

[cont.]

$$\hat{\Gamma}_\alpha(\mathbf{x}, T) = \hat{\Gamma}_\alpha^0(\mathbf{x}, T) + \alpha(T - T_0).$$

The $u_0^{*(\alpha)}$, $s_0^{*(\alpha)}$ are internal energies and entropies of the phases, while $\rho = \rho_{(\alpha)}^0$ ($\alpha = 1, 2$) is the density at reference temperature T_0 and at stress-free state $\sigma = 0$ (assumed to be the same for both phases). The $\hat{\epsilon}_\alpha(\mathbf{x}, T)$ are the fields of total strain in the respective phases. The eigenstrains $\hat{\Gamma}_\alpha(\mathbf{x}, T)$ of the phases with respect to the reference configuration ($\sigma = 0, T = T_0$) might, in general, be of various physical origin. In the present paper we explicitly take into account the strains originating from thermal expansion of the material and eigenstrains originating from thermoelastic phase transformation ($\hat{\Gamma}_\alpha^0(\mathbf{x}, T)$). Please note that we have made an assumption that phase transformation eigenstrains does depend on temperature. This assumption is well justified for the case of the so-called R-phase transformation [7]. In the case of monoclinic martensitic transformation in the pseudoelastic range of SMA materials behavior, the $\hat{\Gamma}_\alpha^0$ may be adopted to be independent of temperature. The dependence of $\hat{\Gamma}_\alpha^0$ on location in the RVE results from the assumption that RVE domain will usually embrace the austenitic phase and many martensitic variants. In our present investigations, the microstructure of the RVE domain is assumed to be known and fixed, being otherwise totally arbitrary. We neglect at the moment any eigenstrains originating from, e.g. the plastic deformations induced as a result of the SMA training procedure. The training procedure of SMA materials is a standard step in obtaining so-called two-way shape memory effect.

In the sequel $\pi_0^f(T)$ denotes the difference of free energy micro-potentials of the phases at the stress-free state ($\sigma = 0$),

$$(4.2) \quad \pi_0^f(T) = \phi_{(1)}^0 - \phi_{(2)}^0 = \Delta u^* - T \Delta s^*, \quad \Delta u^* = u_0^{*(1)} - u_0^{*(2)},$$

$$\Delta s^* = s_0^{*(1)} - s_0^{*(2)}.$$

The mean free energy macro-potential of RVE (per unit of volume) may be expressed with the aid of the meso-scale state variables as follows,

$$(4.3) \quad \rho\Phi = \langle \rho\phi \rangle_{v_0} = \rho\Phi_0 + \rho\Phi_m,$$

$$\rho\Phi_0 = \rho(z_1\phi_{(1)}^0(T) + z_2\phi_{(2)}^0(T)) = c[T - T_0 - T \ln(T/T_0)]$$

$$+ u_0^{*(1)} - T s_0^{*(1)} - z_2\pi_0^f(T),$$

$$\begin{aligned}
 (4.3) \\
 [\text{cont.}] \quad \rho\Phi_m &= 0.5 \left[z_1 \left\langle \hat{\boldsymbol{\sigma}}(\mathbf{x}, T) \cdot \mathbf{M}_1 \hat{\boldsymbol{\sigma}}_\alpha(\mathbf{x}, T) \right\rangle_{v_1} \right. \\
 &\quad \left. + z_2 \left\langle \hat{\boldsymbol{\sigma}}(\mathbf{x}, T) \cdot \mathbf{M}_2 \hat{\boldsymbol{\sigma}}(\mathbf{x}, T) \right\rangle_{v_2} \right], \\
 \hat{\boldsymbol{\varepsilon}}(\mathbf{x}, T) &\equiv \hat{\boldsymbol{\varepsilon}}_\alpha(\mathbf{x}, T), \quad \hat{\boldsymbol{\sigma}}(\mathbf{x}, T) \equiv \hat{\boldsymbol{\sigma}}_\alpha(\mathbf{x}, T), \quad \text{for } \mathbf{x} \in V_\alpha, \\
 &\hspace{25em} V_0 \equiv V_1 + V_2, \\
 z_\alpha &\equiv V_\alpha/V_0, \quad z_1 + z_2 \equiv 1, \quad \langle (\cdot) \rangle_\alpha \equiv \frac{1}{V_\alpha} \int_{V_\alpha} (\cdot) dV.
 \end{aligned}$$

where Φ_0 is an average free energy of mixture of phases at a stress-free state, Φ_m is an average elastic energy stored in macro-element as a result of the conditions applied on its boundary. The $\hat{\boldsymbol{\sigma}}_\alpha(\mathbf{x}, T)$ are the stress fields in the volumes of respective phases V_α , $\alpha = 1, 2$. The symbol V_0 denotes total volume of a macro-element. The definitions (4.3)₄ are only used to shorten the notation. In the case of shape memory alloys, due to a slight difference in density of austenitic and martensitic phases, the mass fractions z_α and volume fractions v_α of the respective phases can be identified.

The elastic energy Φ_m is here of special interest. It can be determined with the aid of solution to the following boundary value problem of micro-mechanics. Let us suppose that RVE with volume v_0 is a composite structure of two coherent elastic phases with volumes v_α ($\alpha = 1, 2$), and with an arbitrary but fixed micro-geometry. We assume the RVE to be statistically representative. An RVE is regarded as statistically representative of macro-response of the continuum material neighborhood, if and only if an arbitrary constant macro-stress $\boldsymbol{\Sigma}$ produces, through solution of the relevant boundary value problem with traction boundary condition ($\mathbf{t}^0(\mathbf{x}) = \mathbf{n} \cdot \boldsymbol{\Sigma}$ on ∂V), a macrostrain ($\mathbf{E}^\Sigma = \langle \boldsymbol{\varepsilon}(\mathbf{x}, \boldsymbol{\Sigma}) \rangle_v$) such that when the displacement boundary conditions ($\mathbf{u}^0(\mathbf{x}) = \mathbf{x} \cdot \mathbf{E}^\Sigma$ on ∂V) are imposed instead, then the macrostress ($\langle \boldsymbol{\sigma}(\mathbf{x}, \boldsymbol{\Sigma}) \rangle_v = \boldsymbol{\Sigma}^\Sigma \cong \boldsymbol{\Sigma}$) is obtained, where the equality holds to a given degree of accuracy (see also NEMAT-NASSER and HORI [11]). The direct consequence of statistical representativeness of RVE is that the macrostrain potential $\Psi^\Sigma(\boldsymbol{\Sigma}) \equiv \langle \psi^\Sigma \rangle_v$ and the macrostress potential $\Phi^E(\mathbf{E}) \equiv \langle \phi^E \rangle_v$ correspond to each other in the sense that $\partial(\Psi^\Sigma(\boldsymbol{\Sigma}))/\partial(\boldsymbol{\Sigma}) \cong \mathbf{E}$ while $\partial(\Phi^E(\mathbf{E}))/\partial(\mathbf{E}) \cong \boldsymbol{\Sigma}$, and in accordance with the Legendre transformation $\Psi^\Sigma(\boldsymbol{\Sigma}) + \Phi^E(\mathbf{E}) \cong \boldsymbol{\Sigma} \cdot \mathbf{E}$. This in turn enables us to impose either the traction or the displacement boundary conditions when posing the problem of micro-mechanics aiming at derivation of the particular Helmholtz or Gibbs macro-potential.

In accordance with the thermodynamic formalism, simple derivation of (4.1) with respect to $\hat{\hat{\boldsymbol{\varepsilon}}}(\mathbf{x}, T)$ gives us generalized Hook's laws, which must be obeyed by the phases,

$$(4.4) \quad \hat{\hat{\boldsymbol{\varepsilon}}}(\mathbf{x}, T) = \mathbf{M}_\alpha \hat{\hat{\boldsymbol{\sigma}}}_\alpha(\mathbf{x}, T) + \hat{\hat{\boldsymbol{\Gamma}}}_\alpha(\mathbf{x}, T), \quad \hat{\hat{\boldsymbol{\Gamma}}}_\alpha(\mathbf{x}, T) = \hat{\hat{\boldsymbol{\Gamma}}}_\alpha(T) + \hat{\hat{\boldsymbol{\Gamma}}}_\alpha^d(\mathbf{x}, T),$$

$$\mathbf{x} \in V_\alpha \quad \alpha = 1, 2,$$

$$\hat{\hat{\boldsymbol{\varepsilon}}}_\alpha(\mathbf{x}, T) = \frac{1}{2} \left(\nabla \hat{\hat{\mathbf{u}}}_\alpha + {}^T \nabla \hat{\hat{\mathbf{u}}}_\alpha \right), \quad \hat{\hat{\boldsymbol{\Gamma}}}_\alpha(T) = \left\langle \hat{\hat{\boldsymbol{\Gamma}}}_\alpha(\mathbf{x}, T) \right\rangle_\alpha,$$

$$\left\langle \hat{\hat{\boldsymbol{\Gamma}}}_\alpha^d(\mathbf{x}, T) \right\rangle_\alpha \equiv 0.$$

where $\hat{\hat{\boldsymbol{\Gamma}}}_\alpha(T)$ is the volume average of the local eigenstrain field $\hat{\hat{\boldsymbol{\Gamma}}}_\alpha(\mathbf{x}, T)$ over the domain of the phase α , while $\hat{\hat{\boldsymbol{\Gamma}}}_\alpha^d(\mathbf{x}, T)$ is the field of deviations of the eigenstrain field from the respective mean value $\hat{\hat{\boldsymbol{\Gamma}}}_\alpha(T)$. The fields $\hat{\hat{\boldsymbol{\sigma}}}(\mathbf{x}, T)$ and $\hat{\hat{\boldsymbol{\varepsilon}}}(\mathbf{x}, t)$ can be discontinuous on the phase boundaries.

We are searching for the displacement field $\hat{\hat{\mathbf{u}}}(\mathbf{x}, T)$ continuous in the whole domain of RVE, which at a fixed microgeometry, prescribed fields of eigenstrain $\hat{\hat{\boldsymbol{\Gamma}}}_\alpha(\mathbf{x}, T)$ and prescribed uniform boundary condition on the surface ∂V of the macro-element,

$$(4.5) \quad \mathbf{n} \cdot \hat{\hat{\boldsymbol{\sigma}}}(\mathbf{x}, T) \Big|_{\partial V} = \mathbf{n} \cdot \boldsymbol{\sigma}^{(z)}.$$

(where $\boldsymbol{\sigma}^{(z)} = \text{const}$ denotes the prescribed uniform stress. Naturally, it is equal to the average stress in the RVE. It denotes also macroscopic stress in the investigated macroscopic material point), gives after substitution into (4.4), the stress fields $\hat{\hat{\boldsymbol{\sigma}}}_\alpha(\mathbf{x}, T)$, which identically satisfy the mechanical equilibrium equations,

$$(4.6) \quad \text{div}(\hat{\hat{\boldsymbol{\sigma}}}(\mathbf{x}, T)) = 0.$$

Boundary condition (4.5) is commonly accepted in all those derivation where the postulate of local state is assumed to be valid. The postulate asserts that the state of the body in a material point is determined by the arbitrarily small neighborhood around that point (RVE). In that perspective, the postulate of local state tells us that the variations of the local field far from the investigated material point are irrelevant in evaluating its macroscopic state. Hence we may adopt a constant boundary condition on the RVE boundary and neglect any deviations from the mean value on the RVE boundary. Precise formulation of Representative Volume Element Problem requires its infinite dimensions. In actual calculations, the size of the RVE is chosen to be sufficiently large to comprise the

characteristic features of the investigated microstructure and at the same time, sufficiently small to make the postulate of local state valid within acceptable accuracy. The prescribed uniform boundary condition on the RVE boundary in fact predetermines in a natural way the unknown macroscopic state in a material point.

In further part of the present investigation we will keep the temperature T fixed until the very last section. Hence we will not write it explicitly in the further formula believing that it does not produce any misunderstandings. This means at the same time that we will investigate the isothermal problem of elasticity in the next sections. We will return to the full explicit notation with temperature T where necessary.

In general, the problem of elasticity (4.4) – (4.6) posed for actual martensitic microstructures is very difficult. However, when the solution is known, it is very easy to evaluate the elastic energy Φ_m by a simple substitution of the known solution. After the averaging procedure we may obtain an expression for the macroscopic free energy potential (4.3). It will be a function of state parameters measurable on the macro-scale (e.g. phase fractions, averaged eigenstrains, elastic properties of individual phases) as well as some parameters characterizing the RVE microstructure (e.g. the number and direction of martensitic plate layers, etc.).

In the next sections we will try to find a symbolical solution of the micro-mechanical problem posed above, convenient for obtaining a clear structure of the function Φ_m . For that purpose it will be advantageous to divide the solution of the original problem of micro-mechanics into auxiliary problems. This will be done in the next section.

5. Auxiliary boundary value problems of mezo-mechanics

The elastic energy Φ_m strongly depends on actual configuration of the phases emerging during phase transformation, i.e. microstructure of the RVE. The two idealized situations can be distinguished leading to the lower and upper estimates of elastic energy Φ_m , so-called REUSS and VOIGT estimates, respectively (see, e.g. HILL ([5])). In the case of VOIGT estimate it is assumed that average strains in individual phases are equal, what corresponds to a mechanical model of the RVE consisting of a set of springs connected in parallel under load. Alternatively we may imagine that this situation corresponds to the macro-element microstructure composed of flat martensitic and possibly austenitic plates oriented in parallel to the applied stress vector. Then the obtained value of energy constitutes the upper estimate of the real value of RVE elastic energy. In the case of Reuss estimate it is assumed that the average stresses in an individual phases are equal.

This supposition corresponds to a mechanical model of the RVE consisting of a set of springs connected in series under loading force or a microstructure composed of martensitic plates and possibly austenitic plates oriented perpendicularly to the applied stress vector. The Reuss model gives a lower estimate of the actual elastic energy of the RVE. Usually none of these microstructures appears in reality and the actual elastic energy of RVE lies somewhere between the REUSS and VOIGT estimate.

The fields of stresses, strains and displacements of original problem (4.4) – (4.6) is now decomposed in a special way,

$$(5.1) \quad \hat{\mathbf{u}}(\mathbf{x}) = \check{\mathbf{u}}(\mathbf{x}) + \boldsymbol{\varepsilon}^{(z)}\mathbf{x}, \quad \hat{\boldsymbol{\varepsilon}}(\mathbf{x}) = \check{\boldsymbol{\varepsilon}}(\mathbf{x}) + \boldsymbol{\varepsilon}^{(z)}, \quad \hat{\boldsymbol{\sigma}}(\mathbf{x}) = \check{\boldsymbol{\sigma}}(\mathbf{x}) + \boldsymbol{\sigma}^{(z)},$$

$$\boldsymbol{\varepsilon}^{(z)} \equiv \mathbf{M}^V \cdot \boldsymbol{\sigma}^{(z)} + \boldsymbol{\Gamma}^V, \quad \mathbf{M}^V \equiv z_1\mathbf{M}_1 + z_2\mathbf{M}_2.$$

From (4.5) and (5.1)₃ it results that the following condition must be fulfilled,

$$(5.2) \quad \mathbf{n} \cdot \check{\boldsymbol{\sigma}}(\mathbf{x})|_{\partial V} = 0.$$

Thus, the average stress over the total volume of RVE (V_0) from the field $\check{\boldsymbol{\sigma}}(\mathbf{x})$ is equal to zero.

There is an infinite number of additive decompositions in the linear problem of elasticity (4.4) – (4.6). Separation of certain uniform fields of stresses and strains from the solution of the original problem of mezo-mechanics has a twofold application. On the one hand, we want to isolate in the macroscopic free energy potential the terms connected with boundary condition (4.5). On the other hand, we want to obtain the additive decomposition of the total elastic energy of macroelement Φ_m . We will show below that the energy Φ_m may be decomposed into additive form (5.3) linked with additive decomposition expressed by (5.1). The additive decomposition will consist of two parts, the first of which is the lower (Reuss) estimate while the second, in accordance with the result obtained by HILL [5], is always non-negative,

$$(5.3) \quad \rho\Phi_m = \frac{1}{2} \left(\boldsymbol{\varepsilon} - \boldsymbol{\Gamma}^V \right) \cdot \mathbf{L}^R \left(\boldsymbol{\varepsilon} - \boldsymbol{\Gamma}^V \right) + W^*,$$

where $\boldsymbol{\Gamma}^V \equiv \langle \hat{\boldsymbol{\Gamma}}(\mathbf{x}) \rangle_0 = z_1\boldsymbol{\Gamma}_1 + z_2\boldsymbol{\Gamma}_2$ is the average (over the whole RVE volume) phase transformation eigenstrain, while \mathbf{L}^R is the Reuss estimate of the effective tensor of elastic moduli, $\mathbf{L}^R = (\mathbf{M}^V)^{-1}$.

Substituting (5.1) and (4.4)₂ into (4.4)₁ we have,

$$(5.4) \quad \boldsymbol{\varepsilon}^{(z)} + \check{\boldsymbol{\varepsilon}}_a(\mathbf{x}) = \mathbf{M}^V (\check{\boldsymbol{\sigma}}_a(\mathbf{x}) + \boldsymbol{\sigma}^{(z)}) + j_\alpha (\mathbf{M}_2 - \mathbf{M}_1) (\check{\boldsymbol{\sigma}}_a(\mathbf{x}) + \boldsymbol{\sigma}^{(z)})$$

$$+ \boldsymbol{\Gamma}^V + j_\alpha (\boldsymbol{\Gamma}_2 - \boldsymbol{\Gamma}_1) + \hat{\boldsymbol{\Gamma}}_a^d(\mathbf{x})$$

and subsequently,

$$(5.5) \quad \check{\epsilon}_\alpha(\mathbf{x}) = \mathbf{M}_\alpha \check{\sigma}_\alpha(\mathbf{x}) + j_\alpha \Delta^f + \hat{\Gamma}_\alpha^d(\mathbf{x}),$$

$$\Delta^f \equiv (\Gamma_2 - \Gamma_1) + (\mathbf{M}_2 - \mathbf{M}_1) \sigma^{(z)},$$

where the following identities were used,

$$(5.6) \quad \mathbf{M}_\alpha = \mathbf{M}^V + j_\alpha (\mathbf{M}_2 - \mathbf{M}_1), \quad \Gamma_\alpha = \Gamma^V + j_\alpha (\Gamma_2 - \Gamma_1),$$

$$j_1 = -z_2, j_2 = z_1.$$

The expression for Δ^f can also be expressed in terms of $\epsilon^{(z)}$ using the identities shown below,

$$(5.7) \quad (\Gamma_2 - \Gamma_1) \equiv (\mathbf{L}^U)^{-1} (\mathbf{L}_2 \Gamma_2 - \mathbf{L}_1 \Gamma_1 + (\mathbf{L}_1 - \mathbf{L}_2) \Gamma^V),$$

$$(\mathbf{M}_2 - \mathbf{M}_1) (\mathbf{M}^V)^{-1} \equiv (\mathbf{L}^U)^{-1} (\mathbf{L}_1 - \mathbf{L}_2) \quad \text{where} \quad \mathbf{L}^U = z_2 \mathbf{L}_1 + z_1 \mathbf{L}_2.$$

Combining (5.7) with (5.1)₂ we obtain,

$$(5.8) \quad \Delta^f = (\mathbf{L}^U)^{-1} \Sigma^f, \quad \Sigma^f \equiv \Sigma^\Gamma + \mathbf{L}^d \epsilon^{(z)}, \quad \Sigma^\Gamma \equiv \mathbf{L}_2 \Gamma_2 - \mathbf{L}_1 \Gamma_1,$$

$$\mathbf{L}^d \equiv (\mathbf{L}_1 - \mathbf{L}_2).$$

In view of (5.5)₁, (5.2) and (4.6), the primary problem of micro-mechanics has been reduced to the following problem,

$$(5.9) \quad \check{\epsilon}_\alpha(\mathbf{x}) = \mathbf{M}_\alpha \check{\sigma}_\alpha(\mathbf{x}) + \hat{\Gamma}_\alpha^*(\mathbf{x}), \quad \text{div}(\check{\sigma}) = 0, \quad \check{\mathbf{t}}(\mathbf{x})|_{\partial V} = 0,$$

$$\hat{\Gamma}_\alpha^*(\mathbf{x}) \equiv j_\alpha \Delta^f + \hat{\Gamma}_\alpha^d(\mathbf{x}).$$

When the solution of problem (5.9) is known, then the solution of primary problem (4.4) – (4.6) can be immediately found with the aid of (5.1). The decomposition (5.1) leads to the following division of macro-element elastic energy,

$$(5.10) \quad \rho \bar{\mathcal{E}}_m = \frac{1}{2} \left[z_1 \left\langle \left(\check{\sigma}(\mathbf{x}) + \sigma^{(z)} \right) \cdot \mathbf{M}_1 \left(\check{\sigma}(\mathbf{x}) + \sigma^{(z)} \right) \right\rangle_1 \right. \\ \left. + z_2 \left\langle \left(\check{\sigma}(\mathbf{x}) + \sigma^{(z)} \right) \cdot \mathbf{M}_2 \left(\check{\sigma}(\mathbf{x}) + \sigma^{(z)} \right) \right\rangle_2 \right] \\ = \frac{1}{2} \left[z_1 \left\langle \check{\sigma}(\mathbf{x}) \cdot \mathbf{M}_1 \check{\sigma}(\mathbf{x}) \right\rangle_1 + z_2 \left\langle \check{\sigma}(\mathbf{x}) \cdot \mathbf{M}_2 \check{\sigma}(\mathbf{x}) \right\rangle_2 + \sigma^{(z)} \cdot \mathbf{M}^V \sigma^{(z)} \right],$$

since

$$\begin{aligned} 2 \left(z_1 \langle \check{\sigma}(\mathbf{x}) \rangle_1 \cdot \mathbf{M}_1 \sigma^{(z)} + z_2 \langle \check{\sigma}(\mathbf{x}) \rangle_2 \cdot \mathbf{M}_2 \sigma^{(z)} \right) \\ = 2(-z_1 z_2 + z_1 z_2) (\Delta \varepsilon - \Delta^f) \cdot \sigma^{(z)} = 0, \end{aligned}$$

where in the above formulae the following relations were used (see (5.9)),

$$\begin{aligned} (5.11) \quad \langle \check{\sigma}(\mathbf{x}) \rangle_1 &= -z_2 \mathbf{L}_1 (\Delta \varepsilon - \Delta^f), \quad \langle \check{\sigma}(\mathbf{x}) \rangle_2 = z_1 \mathbf{L}_2 (\Delta \varepsilon - \Delta^f), \\ \langle \check{\varepsilon}(\mathbf{x}) \rangle_\alpha &= \langle \check{\varepsilon}(\mathbf{x}) \rangle_0 + j_\alpha \Delta \varepsilon, \quad \Delta \varepsilon = \langle \check{\varepsilon}(\mathbf{x}) \rangle_2 - \langle \check{\varepsilon}(\mathbf{x}) \rangle_1, \\ \langle \check{\sigma}(\mathbf{x}) \rangle_0 &= 0, \quad \langle \hat{\Gamma}_\alpha^d(\mathbf{x}) \rangle_\alpha = 0. \end{aligned}$$

After substituting (5.1)₂ into (5.10)₂, the explicit form of energy W^* appearing in (5.3) is obtained,

$$(5.12) \quad W^* = \frac{1}{2} \left[z_1 \langle \check{\sigma}(\mathbf{x}) \cdot \mathbf{M}_1 \check{\sigma}(\mathbf{x}) \rangle_1 + z_2 \langle \check{\sigma}(\mathbf{x}) \cdot \mathbf{M}_2 \check{\sigma}(\mathbf{x}) \rangle_2 \right] \geq 0.$$

Hereby, we have proved that with the additive decomposition (5.1), additive decomposition of elastic energy (5.3) is linked. It is worth noting that decomposition (5.3) is quite arbitrary. At the moment it has the drawback that energy W^* depends explicitly on $\varepsilon^{(z)}$. We will correct this deficiency later by introducing the energy W^{**} .

As it can be seen from (5.9) and (5.12), the energy W^* can be interpreted as an elastic energy of specific comparative macro-element with no force loads on external walls, and stored in the effect of operation of the "Ersatz" eigenstrains $\hat{\Gamma}_\alpha^*$ defined by (5.9)₂. The comparative macro-element has the same microstructure and material properties as the actual macro-element.

Let us return to the problem (5.9). The solution of this problem may also be expressed as a sum of two auxiliary solutions in a manner similar to that applied in the case of the original problem,

$$\begin{aligned} (5.13) \quad \check{\mathbf{u}} &= \check{\mathbf{u}}'(\mathbf{x}) + \check{\mathbf{u}}''(\mathbf{x}), \quad \check{\varepsilon}(\mathbf{x}) = \check{\varepsilon}'(\mathbf{x}) + \check{\varepsilon}''(\mathbf{x}), \\ \check{\sigma}(\mathbf{x}) &= \check{\sigma}'(\mathbf{x}) + \check{\sigma}''(\mathbf{x}), \\ \check{\varepsilon}'_\alpha(\mathbf{x}) &= \mathbf{M}_\alpha \check{\sigma}'_\alpha(\mathbf{x}) + j_\alpha \Delta^f, \quad \check{\varepsilon}''_\alpha(\mathbf{x}) = \mathbf{M}_\alpha \check{\sigma}''_\alpha(\mathbf{x}) + \hat{\Gamma}_\alpha^d(\mathbf{x}), \\ \check{\mathbf{t}}'(\mathbf{x})|_{\partial V} &= \check{\mathbf{t}}''(\mathbf{x})|_{\partial V} = 0. \end{aligned}$$

The physical reason for appearance of non-vanishing fields $\check{\sigma}''_\alpha(\mathbf{x})$, $\check{\varepsilon}''_\alpha(\mathbf{x})$, can be the formation (during phase transformation) of variously oriented mismatching variants of martensitic plates, e.g. due to kinematic constraints. These fields do

not depend on the average values Γ_α of eigenstrains of particular phases, nor on the average total stress $\sigma^{(z)}$ prescribed by the boundary condition.

The following relations are valid due to the boundary conditions of auxiliary problems (5.13) (see also NEMAT-NASSER and HORI [11]),

$$(5.14) \quad \begin{aligned} \langle \check{\sigma}'(\mathbf{x}) \cdot \check{\varepsilon}'(\mathbf{x}) \rangle_0 &= \langle \check{\sigma}''(\mathbf{x}) \cdot \check{\varepsilon}'(\mathbf{x}) \rangle_0 = \langle \check{\sigma}'(\mathbf{x}) \cdot \check{\varepsilon}''(\mathbf{x}) \rangle_0 \\ &= \langle \check{\sigma}''(\mathbf{x}) \cdot \check{\varepsilon}''(\mathbf{x}) \rangle_0 = 0, \\ \langle \sigma(\mathbf{x}) \cdot \varepsilon(\mathbf{x}) \rangle_0 &\equiv \frac{1}{V_0} \int_{V_0} \sigma(\mathbf{x}) \cdot \varepsilon(\mathbf{x}) dV. \end{aligned}$$

This means that the average work of stresses on the corresponding strains calculated over the total volume of the macro-element is always equal to zero. The above relations result directly from application of the Gauss theorem, the mechanical equilibrium conditions and boundary conditions of the auxiliary problems. In the sequel, the following notation is used,

$$(5.15) \quad \begin{aligned} \varepsilon'_\alpha &= \langle \check{\varepsilon}'_\alpha(\mathbf{x}) \rangle_\alpha, & \varepsilon''_\alpha &= \langle \check{\varepsilon}''_\alpha(\mathbf{x}) \rangle_\alpha, & \Delta\varepsilon' &= \varepsilon'_2 - \varepsilon'_1, & \Delta\varepsilon'' &= \varepsilon''_2 - \varepsilon''_1, \\ \sigma'_\alpha &= \langle \check{\sigma}'_\alpha(\mathbf{x}) \rangle_\alpha, & \sigma''_\alpha &= \langle \check{\sigma}''_\alpha(\mathbf{x}) \rangle_\alpha, & \Delta\sigma' &= \sigma'_2 - \sigma'_1, & \Delta\sigma'' &= \sigma''_2 - \sigma''_1. \end{aligned}$$

Averaging (5.13)₂ over the total volume of RVE and using (5.13)₁ and (5.11)₂ yields,

$$(5.16) \quad \begin{aligned} \Delta\sigma' &= \mathbf{L}^U(\Delta\varepsilon' - \Delta\mathbf{f}), & \Delta\sigma'' &= \mathbf{L}^U \Delta\varepsilon'', \\ \Delta\sigma &= \Delta\sigma' + \Delta\sigma'', & \Delta\varepsilon &= \Delta\varepsilon' + \Delta\varepsilon'', & \Delta\sigma &= \mathbf{L}^U(\Delta\varepsilon - \Delta\mathbf{f}). \end{aligned}$$

The above relations will be used in the next section.

6. The accommodation energy W^{**}

The decomposition of energy W^* (5.12) can be performed in the same way as in the case of energy Φ_m (formula (5.10)),

$$(6.1) \quad \begin{aligned} W^* &= \frac{1}{2} \left[z_1 \left\langle (\check{\sigma}' + \check{\sigma}'') \cdot \mathbf{M}_1(\check{\sigma}' + \check{\sigma}'') \right\rangle_1 \right. \\ &\quad \left. + z_2 \left\langle (\check{\sigma}' + \check{\sigma}'') \cdot \mathbf{M}_2(\check{\sigma}' + \check{\sigma}'') \right\rangle_2 \right]. \end{aligned}$$

Then using the relations (5.13)₂ for $\mathbf{M}_\alpha \check{\boldsymbol{\sigma}}_\alpha(\mathbf{x})$ and simplifying the obtained formula by means of relations (5.14), we have,

$$(6.2) \quad W^* = \frac{1}{2} \left[z_1 z_2 \left\langle \check{\boldsymbol{\sigma}}'_1(\mathbf{x}) \right\rangle_1 \cdot \Delta^f - z_1 z_2 \left\langle \check{\boldsymbol{\sigma}}'_2(\mathbf{x}) \right\rangle \cdot \Delta^f \right. \\ \left. - z_1 \left\langle \check{\boldsymbol{\sigma}}''_1(\mathbf{x}) \cdot \hat{\Gamma}_1^d(\mathbf{x}) \right\rangle_1 - z_2 \left\langle \check{\boldsymbol{\sigma}}''_2(\mathbf{x}) \cdot \hat{\Gamma}_2^d(\mathbf{x}) \right\rangle_2 \right. \\ \left. + 2z_1 \left\langle \check{\boldsymbol{\sigma}}''_1(\mathbf{x}) \cdot (\check{\boldsymbol{\xi}}'_1(\mathbf{x}) + z_2 \Delta^f) \right\rangle_1 + 2z_2 \left\langle \check{\boldsymbol{\sigma}}''_2(\mathbf{x}) \cdot (\check{\boldsymbol{\xi}}'_2(\mathbf{x}) - z_1 \Delta^f) \right\rangle_2 \right].$$

Next, using (5.8)₁, (5.15) and taking advantage of the properties (5.16), we obtain,

$$(6.3) \quad 2W^* = -z_1 z_2 \Sigma^f \cdot (\Delta \boldsymbol{\varepsilon}' + 2\Delta \boldsymbol{\varepsilon}'' - \Delta^f) - z_1 \left\langle \check{\boldsymbol{\sigma}}''_1(\mathbf{x}) \cdot \hat{\Gamma}_1^d(\mathbf{x}) \right\rangle_1 \\ - z_2 \left\langle \check{\boldsymbol{\sigma}}''_2(\mathbf{x}) \cdot \hat{\Gamma}_2^d(\mathbf{x}) \right\rangle_2.$$

The solution of the problem marked by the "prime" symbol can be written in the following symbolic form (see also HILL [5]),

$$(6.4) \quad \check{\boldsymbol{\xi}}'_\alpha(\mathbf{x}) = \mathcal{M}_\alpha(\mathbf{x}) \Sigma^f, \quad \Delta \boldsymbol{\varepsilon}' = \mathcal{M} \Sigma^f, \quad \mathcal{M} = \langle \mathcal{M}_2(\mathbf{x}) \rangle_2 - \langle \mathcal{M}_1(\mathbf{x}) \rangle_1,$$

where concentration tensors \mathcal{M}_α depend in general on the parameters representing microstructure, phase fractions and elastic moduli, etc..

The average partial strains (second-order strains) constituting the solution of the problem (4.4) – (4.6) can be now expressed as follows,

$$(6.5) \quad \hat{\boldsymbol{\varepsilon}}_\alpha = \boldsymbol{\varepsilon}^{(z)} + j_\alpha (\mathcal{M} \Sigma^f + \Delta \boldsymbol{\varepsilon}'').$$

There exists a direct relation between the tensor \mathcal{M} and the classical Hill's concentration tensors. The general averaged solution of the original problem investigated can be presented in the form,

$$(6.6) \quad \hat{\boldsymbol{\varepsilon}}_\alpha = \langle \hat{\boldsymbol{\varepsilon}}_\alpha(\mathbf{x}) \rangle_\alpha = \mathbf{A}_\alpha \boldsymbol{\varepsilon}^{(z)} + \mathbf{D}_{\alpha 1} \Gamma_1 + \mathbf{D}_{\alpha 2} \Gamma_2.$$

Using (5.8) and assuming $\hat{\Gamma}_\alpha^d(\mathbf{x}) \equiv 0$ ($\Delta \boldsymbol{\varepsilon}'' \equiv 0$), it can be easily observed by comparison of (6.5) and (6.6), that the following relations are valid,

$$(6.7) \quad \mathbf{A}_\alpha = \mathbf{I} + j_\alpha \mathcal{M}(\mathbf{L}_1 - \mathbf{L}_2), \quad \mathbf{D}_{\alpha 1} = -j_\alpha \mathcal{M} \mathbf{L}_1, \quad \mathbf{D}_{\alpha 2} = j_\alpha \mathcal{M} \mathbf{L}_2.$$

Because the Hill's concentration tensors $\mathbf{A}_\alpha, \mathbf{D}_{\alpha 1}, \mathbf{D}_{\alpha 2}$ depend on the single fourth order tensor \mathcal{M} , then whenever one of them is known, then the other one can be immediately determined, in view of the relations (6.7).

The relations (6.4) yield,

$$(6.8) \quad W^* = \frac{1}{2} z_1 z_2 \Sigma^f \cdot ((\mathbf{L}^U)^{-1} - \mathcal{M}) \Sigma^f + [z_1 W_1 + z_2 W_2] - z_1 z_2 \Sigma^f \cdot \mathcal{N},$$

$$\mathcal{N} \equiv \Delta \varepsilon'', \quad W_1 \equiv -\frac{1}{2} \langle \check{\sigma}_1''(\mathbf{x}) \cdot \hat{\Gamma}_1^d(\mathbf{x}) \rangle_1,$$

$$W_2 \equiv -\frac{1}{2} \langle \check{\sigma}_2''(\mathbf{x}) \cdot \hat{\Gamma}_2^d(\mathbf{x}) \rangle_2.$$

When deviations from the average values of the eigenstrains in the phases $\hat{\Gamma}_\alpha^d(\mathbf{x}) \equiv 0$, then the terms W_α and \mathcal{N} are also identically equal to zero and the first term appearing on the right hand side of (6.8)₁ is the only non-zero term. It should be observed that tensors \mathcal{M} , \mathcal{N} and energies W_α do not depend on $\sigma^{(z)}$ and on Γ_α , they are however functions of the macro-element micro-geometry, elastic moduli \mathbf{L}_α and phase fractions z_α .

The terms W_α (6.8)₂ can be expressed in the form where parts linearly proportional to the phase mass fractions z_α are explicitly separated,

$$(6.9) \quad W_\alpha = W_\alpha^* + j_\alpha W_\alpha^0,$$

where the terms $W_\alpha^* \geq 0$ do not depend linearly on z_α .

Then the expression for energy W^* takes the form,

$$(6.10) \quad W^* = z_1 z_2 \rho \Phi_{it} + z_1 W_1^* + z_2 W_2^* \geq 0$$

$$\rho \Phi_{it} \equiv \frac{1}{2} \Sigma^f \cdot ((\mathbf{L}^U)^{-1} - \mathcal{M}) \Sigma^f - \Sigma^f \cdot \mathcal{N} + \Delta W^0, \quad \Delta W^0 = W_2^0 - W_1^0.$$

Using (4.3), (5.3) and (6.10), the macroscopic free energy potential of SMA macro-element may be expressed as follows,

$$(6.11) \quad \rho \Phi = \frac{1}{2} (\varepsilon^{(z)} - \Gamma^V) \cdot \mathbf{L}^R (\varepsilon^{(z)} - \Gamma^V) + z_1 z_2 \rho \Phi_{it} + z_1 W_1^* + z_2 W_2^* + \rho \Phi_0(T).$$

By direct differentiation of the free energy function Φ with respect to $\varepsilon^{(z)}$, we can obtain the thermo-mechanical constitutive relations for the SMA macro-element. They are valid when the conditions for elastic behavior of the material

are fulfilled (no phase transformation or dissipative change of microstructure). They take the following form,

$$\begin{aligned} \sigma^{(z)} &\equiv \partial(\rho\Phi)/\partial\varepsilon^{(z)} = \mathbf{L}^{ef} \varepsilon^{(z)} + \varepsilon^{pe}, \\ (6.12) \quad \mathbf{L}^{ef} &\equiv \mathbf{L}^R + z_1 z_2 \mathbf{L}^d \left((\mathbf{L}^U)^{-1} - \mathcal{M} \right) \mathbf{L}^d, \\ \varepsilon^{pe} &\equiv \left(\mathbf{L}^{ef} \right)^{-1} \left[\mathbf{L}^R \Gamma^V - z_1 z_2 \left(\mathbf{L}^d \cdot \left((\mathbf{L}^U)^{-1} - \mathcal{M} \right) \Sigma^\Gamma - \mathbf{L}^d \mathcal{N} \right) \right]. \end{aligned}$$

Neither the effective elastic tensor \mathbf{L}^{ef} nor the effective (macroscopic) phase transformation eigenstrain tensor ε^{pe} does depend on $\varepsilon^{(z)}$. In the case when $\mathbf{L}_1 = \mathbf{L}_2$, the above expressions can be considerably simplified to give,

$$(6.13) \quad \mathbf{L}^{ef} \equiv \mathbf{L}, \quad \varepsilon^{pe} \equiv \Gamma^V, \quad \sigma^{(z)} \equiv \mathbf{L} \left(\varepsilon^{(z)} - \Gamma^V \right).$$

A more detailed discussion of some special cases will be presented in the next section. We may now rewrite the expression for the free energy of the SMA macro-element in the most convenient form,

$$(6.14) \quad \rho\Phi = \frac{1}{2} (\varepsilon^{(z)} - \varepsilon^{pe}) \cdot \mathbf{L}^{ef} (\varepsilon^{(z)} - \varepsilon^{pe}) + W^{**} + \rho\Phi_0(T).$$

The formula (6.14) constitutes the central result of the present paper.

Comparing (6.11) and (6.14) and using inequality (5.12) it is easy to show that the following inequality holds,

$$(6.15) \quad W^{**} \equiv z_1 z_2 \rho \Phi_{it}^* + z_1 W_1^* + z_2 W_2^* \geq 0,$$

while

$$\begin{aligned} (6.16) \quad \rho\Phi_{it}^* &\equiv \frac{1}{2} \varepsilon^{pe} \mathbf{L}^d \left((\mathbf{L}^U)^{-1} - \mathcal{M} \right) \mathbf{L}^d \Gamma^V \\ &\quad + \frac{1}{2} \left(\Gamma^V + \varepsilon^{pe} \right) \left(\mathbf{L}^d \left((\mathbf{L}^U)^{-1} - \mathcal{M} \right) \Sigma^\Gamma \right. \\ &\quad \left. - \mathbf{L}^d \mathcal{N} \right) + \frac{1}{2} \Sigma^\Gamma \left((\mathbf{L}^U)^{-1} - \mathcal{M} \right) \Sigma^\Gamma - \Sigma^\Gamma \mathcal{N} + \Delta W^0. \end{aligned}$$

Please note that the energy Φ_{it}^* defined by (6.16) does not depend on $\varepsilon^{(z)}$.

The general form of function Φ (formula (6.14)) derived in this paper is valid for an arbitrary microstructure. The weak point is here the fact that the functional dependence of the objects \mathcal{M} , \mathcal{N} and W_α on particular micro-structural geometry is not known, neither is their evolution with applied external thermo-mechanical loads (e.g. ε and T). In general, the dependence of average phase transformation eigenstrains Γ_α on the temperature or mechanical load is also

not known. Hence the expression for free energy potential (6.14) is in fact quite formal.

It would be interesting for the reader to see how this result may be used to obtain the explicit free energy potential applicable for construction of the SMA materials incremental constitutive model. Such a model has been already constructed. It is the so-called R_L model of SMA pseudoelastic behavior proposed by RANIECKI, LEXCELLENT and TANAKA in [18] and later extended by RANIECKI and LEXCELLENT in [17]. We will specify below the simplifications that had to be introduced into the formula (6.14) in order to obtain the form of free energy function used in the R_L model of the SMA materials behavior,

i) It was assumed that both the phases constitute isotropic elastic solids with the same elastic moduli, the same thermal expansion coefficient α and the same specific heats c . Then the Reuss and Voigt estimates, as well as the tensors \mathbf{L}^{ef} , \mathbf{L}^R , \mathbf{L}^U , reduce to the one isotropic tensor of elastic moduli \mathbf{L} ($\mathbf{L}^d \equiv 0$).

ii) The eigenstrains were proposed in the form,

$$(6.17) \quad \Gamma_1 = \alpha_0(T - T_0)\mathbf{1}; \quad \Gamma_2 = \alpha_0(T - T_0)\mathbf{1} + \mathbf{k},$$

where $\mathbf{1}$ denotes the second order unit tensor, and \mathbf{k} constitutes an approximation of the overall average strain connected with thermoelastic phase transformation. This assumption leads to the following estimation of the tensor: $\boldsymbol{\varepsilon}^{pe} = \Gamma^V = \alpha_0(T - T_0)\mathbf{1} + z_2\mathbf{k}$. Moreover, the authors of the R_L model have accepted that the trace of the phase distortion tensor \mathbf{k} is always zero, and that it is always collinear with the total strain deviator in accordance with the following formula,

$$(6.18) \quad \mathbf{k} = \eta \bar{\boldsymbol{\varepsilon}} / \varepsilon, \quad \varepsilon = (\bar{\boldsymbol{\varepsilon}} \cdot \bar{\boldsymbol{\varepsilon}})^{1/2}, \quad \text{tr}(\mathbf{k}) = 0,$$

where η is an amplitude of pseudoelastic flow in simple tension.

iii) The energy of internal interactions between the phases $z_1 z_2 \rho \Phi_{it}^*$ (see (6.16)) was proposed in the form of a linear function of temperature,

$$(6.19) \quad \Phi_{it}^*(T) = \bar{u}_0 - T \bar{s}_0,$$

where \bar{u}_0, \bar{s}_0 are material constants, which are to be identified on the basis of the existing experimental data. Hence, as a first guess in the R_L model, the influence of changing microstructure and mass fractions on the tensors $((\mathbf{L}^U)^{-1} - \mathcal{M})$, \mathcal{N} and scalar ΔW^0 has been neglected. Note that when $\mathbf{L}^d \equiv 0$ then in formula (6.16) only the last three terms are non-zero.

iv) It was additionally assumed that the term W_1^* is negligible, while $W_2^* = \bar{u}_0^{*(1)} - T \bar{s}_0^{*(1)}$ is a linear function of temperature, this assumption allows us to include subsequently the terms connected with W_2^* i.e. $\bar{u}_0^{*(2)}, \bar{s}_0^{*(2)}$ into the terms $u_0^{*(2)}, s_0^{*(2)}$ representing the internal energy and entropy of the martensitic phase

formation in the reference state ($\sigma = 0, T = T_0$). The last operation allows us to use negative interaction energy $z_1 z_2 \rho \bar{\Phi}_{it}^*$ during modeling of the R-phase transformation. We will present a more detailed discussion on that subject in the next section.

After substitution of the simplifying assumptions from **i**) to **iv**) into the formula (6.14) we obtain the form of free energy function proposed in paper [18],

$$\begin{aligned} \bar{\Phi}_c &= (\varepsilon - \varepsilon^{pe}) \cdot \mathbf{L}(\varepsilon - \varepsilon^{pe})/2 - (T - T_0)\alpha_0 \cdot \mathbf{L}(\varepsilon - \varepsilon^{pe}) \\ &\quad + \phi^*(T, z), \\ (6.20) \quad \phi^*(T, z) &\equiv c(T - T_0) - cT \ln(T/T_0) + u_0^{*(1)} - Ts_0^{*(1)} - z\pi_0^f(T) \\ &\quad + \phi_{it}(T)(1 - z)z, \\ \varepsilon^{pe}(z, \mathbf{k}) &= \eta z \bar{\varepsilon} / \varepsilon. \end{aligned}$$

We will omit here the discussion on how to construct the SMA constitutive model using $\bar{\Phi}_c$, and its validation with the macroscopic experimental evidence obtained for SMA materials, sending the interested readers to the papers [17, 18, 7].

7. Discussion and conclusions

In the previous section we have obtained the expression for macroscopic free energy function assumed to be valid for shape memory alloys in their pseudoelastic range of behavior (6.14). The first term appearing on the right hand side of formula (6.14) is "classical". It is quite well known from, e.g. the theory of plasticity. It represents a response of the system loaded mechanically in the form of elastic energy storage, which is fully recoverable under unloading. The strains ε^{pe} represent in general the inelastic strains and may be of various origins (phase transformation, reorientation, plasticity, and other non-mechanical fields, e.g. magnetic or thermal).

The last term on the right hand side of formula (6.14) is also quite classical. It can be used to describe the thermal phenomena – taking place in the material, such as e.g. heat capacity or entropy change of the SMA macro-element during the loading or unloading processes.

The most interesting term appearing in the formula (6.14) is the term W^{**} that we called the accommodation energy. It is defined by the formula (6.15) and is always non-negative. The thermo-elastic martensitic transformation takes place in a SMA macro-element upon reaching certain critical conditions. The austenite-martensite microstructure starts to appear adapting to the external

load. By adaptation we mean minimization of free energy of the macro-element "as much as possible". We will explain what we mean by that thereafter. The thermo-elastic martensitic transformation is coherent. This constraint must be fulfilled at all times. For some special austenite-martensite microstructures it is possible without using any force. In such cases the microstructure is like a set of perfectly matching "puzzle" pieces. We may say that "ideal accommodation of microstructure to the applied loading" takes place. This expression can be often found in the literature devoted to physical foundations of metallurgy. We may express this special situation in precise mathematical terms of the problem of mezo-mechanics investigated in the present paper.

Let us assume that the tensor Δ^f ((5.5)₂ or (5.8)) takes the form of a symmetric diadic of two vectors. Let us also assume that the fields $\hat{\Gamma}_\alpha^d(\mathbf{x})$ (4.4)₂ fulfill the compatibility conditions in the regions of individual phases and geometrical consistency conditions on the inter-phase boundaries. Then the pairs of fields,

$$(7.1) \quad \check{\xi}'_\alpha(\mathbf{x}) = j_\alpha \Delta^f, \quad \check{\sigma}'_\alpha(\mathbf{x}) = 0 \quad \text{and} \quad \check{\xi}''_\alpha(\mathbf{x}) = \hat{\Gamma}_\alpha^d(\mathbf{x}), \quad \check{\sigma}''_\alpha(\mathbf{x}) = 0,$$

make the actual solution of the problem (5.9) (as they identically satisfy the required equilibrium and boundary conditions). Comparing (6.21)₁ with (6.4)₁ we obtain $\mathcal{M} = (\mathbf{L}^U)^{-1}$. Substituting (6.21)₄ into (6.8)₂ we obtain $\mathcal{N} = 0$, $W_\alpha = 0$. Taking advantage of (6.9) we have $\Delta W^0 = 0$, $W_\alpha^* = 0$ for $\alpha = 1, 2$. Using the previous equalities in (6.12) and (6.16) it appears that $\mathbf{L}^{ef} = \mathbf{L}^R$, $\boldsymbol{\varepsilon}^{pe} = \boldsymbol{\Gamma}^V$, $\rho\Phi_{it}^* = 0$. Finally, from (6.15) we obtain $W^{**} = 0$ and the free energy potential (6.14) takes the value of lower (Reuss) estimate $\rho\Phi = \frac{1}{2}(\boldsymbol{\varepsilon}^{(z)} - \boldsymbol{\Gamma}^V) \cdot \mathbf{L}^R(\boldsymbol{\varepsilon}^{(z)} - \boldsymbol{\Gamma}^V) + \rho\Phi_0(T)$ for the considered ideally accommodated microstructure. For the illustrative purposes we may imagine this ideally accommodated "microstructure" as four mono-crystalline martensitic plates composed of one martensitic variant each (no lower level internal martensitic substructure), embedded in mono-crystalline austenite. Such a self-accommodated group of martensitic plates quite often appears for thermally induced thermo-elastic martensite. In the case of self-accommodating group, instead of condition (6.21)₃, a more stringent condition $\check{\xi}''_\alpha(\mathbf{x}) = \hat{\Gamma}_\alpha^d(\mathbf{x}) \equiv 0$ is fulfilled. We may say that when thermally induced groups of self-accommodating martensitic plates are formed then ideal strain accommodation takes place. In such a case not only the energy W^{**} but also the macroscopic total strain of the sample is zero. When "only" $W^{**} = 0$, we may speak about ideal energetic accommodation of the microstructure to the applied load.

In general, it is impossible for the macro-element microstructure to "adapt ideally" to the external load $\boldsymbol{\sigma}^{(z)}$. This means that the conditions (6.21) are not fulfilled in general. In such a case, the compatibility conditions in the regions

of individual phases and the coherency conditions on the inter- and intra- phase boundaries must be enforced by self-equilibrating internal stresses of the second kind. On the macroscopic scale it means that energy $W^{**} > 0$. The energy W^{**} can be termed the energy of unaccommodation of the macro-element microstructure to the prescribed external loading or the coherency energy (MÜLLER and XU [10]). Alternatively it may be termed, as we do it, the accommodation energy since it is this energy, which assures the satisfaction of the compatibility conditions for the actual strain fields and coherence conditions for the displacement fields.

In Section 1 we indicated the paradox in the attempts to describe SMA materials behavior during the R-phase transformation. Identification of the model material parameters led in the case of NiTi alloy undergoing the R-phase transformation to negative values of an interaction energy Φ^{AM} , which seemed somehow impossible on physical grounds. Now we may explain this paradox as follows. The formula (6.15) defines the accommodation energy W^{**} , which as it has been shown above, is always non-negative. The interaction energy $\Phi^{AM} = z_1 z_2 \rho \Phi_{it}^*$ is only a part of the accommodation energy W^{**} . The energy Φ^{AM} may be negative for some special microstructures when at the same time, the terms W_1^* and/or W_2^* are non-negative and $z_1 W_1^* + z_2 W_2^* \geq z_1 z_2 \rho \Phi_{it}^*$. Such a situation occurs when the fields of deviations $\hat{\Gamma}_\alpha^d(\mathbf{x})$ from the mean values of phase eigenstrains are "highly" incompatible (incommensurate). The macroscopic stress-strain curves obtained for NiTi samples undergoing the R-phase transformation (see e.g. Fig. 2), and the investigations presented in the present paper allow to draw conclusion that the reach incommensurate microstructure is forming in the sample undergoing R-phase transformation. In order to coerce the coherence kinematic constraints of the transformation, relatively high energy W_2^* is necessary (in this particular case we may safely assume for not trained NiTi specimens that W_1^* is negligible). The experimental works by MIYAZAKI, WAYMAN [9] confirm this supposition, as they report the formation of incommensurate microstructures in the NiTi samples undergoing R-phase transformation.

The energies W_α^* ($\alpha = 1, 2$) may be completely neglected, e.g. in the case of a CuZnAl mono-crystalline alloy undergoing monoclinic martensitic transformation. This case studied by MÜLLER and XU [10] gave a false impression that the coherency energy $z_1 z_2 \rho \Phi_{it}^*$ introduced by them heuristically constitutes all of the accommodation energy W^{**} .

Although we have managed to explain why and when the interaction energy might be negative, a new open scientific problem has appeared why the actual paths for R-phase transformation deviate from the paths of full thermodynamic equilibrium. In the case of monoclinic martensitic transformation when the interaction energy is positive, it could be explained by instability of full ther-

modynamic equilibrium path. When the interaction energy is negative, the full equilibrium path is stable (see e.g. [18]).

We will discuss one more potential field of application of our research. It is connected with the two-way shape memory effect. At present, a number of different training techniques are applied in order to induce a two-way shape memory effect:

– Deform a sample in fully martensitic state above the plastic yield limit of martensite.

– Deform the sample in austenitic (martensitic) state by application of force, then reduce (increase) the temperature below M_f (above A_f) in the presence of the applied stress.

– Deform the sample in the austenitic state after formation of minute precipitates due to the aging procedure.

The M_f denotes here the martensite finish temperature, while A_f austenite finish temperature. Stabilization and “saturation” of the acquired effect is obtained by application of cyclic mechanical loading at constant temperature, or by cyclic thermal loading at constant (stress, strain), or by application of mixed techniques.

On the micro-scale of observation, all the techniques listed above target at generation of localized centers of internal stresses (possibly uniformly distributed) in the high temperature parent phase. These localized centers of internal stresses are permanent crystallographic lattice defects such as dislocations induced by deformation (techniques one and two mentioned above), stress-induced retained martensite (technique two), precipitates (technique three).

On the macro-scale, the primary target of these procedures is to create self-equilibrated initial stress field within the SMA element in order to enforce particular geometrical path of the forward and reverse phase transformations. The typical apparent macroscopic results of the two-way effect training procedure, consisting in cyclic thermo-mechanical treatment are,

- Existence of the permanent strain at zero stress.
- Shifting of forward critical transformation temperature σ^{AM} towards lower values.
- Serious increase of hardening slope.
- Change in shape and decrease in size of the hysteresis loop.

The evolution resulting from the two-way training procedure of shape memory alloy can be well grasped by comparing the stress-strain curve of Fig. 1 for not trained SMA, and that in Fig. 2 in the paper [15] (which is schematically very similar to the Fig. 2 of the present paper). From the similarity of the stress-strain curves for “R-phase transformation” and “two-way shape memory effect” we can guess that energetically similar phenomena take place in the both cases. We have already revealed in the present section that proper description of the R-phase

transformation requires fulfillment of the inequality $z_1 W_1^* + z_2 W_2^* \geq z_1 z_2 \rho \Phi_{it}^*$. In the case of R-phase transformation it appeared that it was sufficient to assume W_2^* was strictly positive. This term arises from the incompatible eigenstrain fields resulting from the R-phase transformation. In the case of two-way shape memory effect both terms W_α^* ($\alpha = 1, 2$) most probably will have to be assumed to be strictly positive in order to obtain proper modeling description of this effect. On microscopic grounds this statement can be justified by the existence of incompatible strain fields resulting from the training procedure in both phases. They will result from plastic strains, the retained martensite eigenstrains or strains resulting from precipitates in the parent phase, and from incompatible phase transformation eigenstrains in the product phase.

The successful constitutive model of the two-way shape memory effect will require the assumption of the proper form of the terms W_α^* and their evolution. Even when at the beginning they will be zero for a "virgin" SMA sample material ($W_\alpha^* = 0$), after several or several dozens of training cycles, a certain amount of energy will be stored in the modified microstructure of the shape memory macroelement. The self-equilibrated micro-stresses will appear, which do not vanish even when one of the phases completely disappears.

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